

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
 Data File : BG057776.D
 Acq On : 20 Jun 2023 14:49
 Operator : CG/JU
 Sample : 03287-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 OK-1-061523

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057776.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.032	326	331	338	rBV	72410	112025	4.87%	0.635%
2	5.502	402	411	421	rBV	888387	1406427	61.20%	7.976%
3	7.089	673	681	697	rVB	886491	1508074	65.63%	8.552%
4	7.929	815	824	831	rBV	153743	252591	10.99%	1.432%
5	9.092	1013	1022	1030	rBV	524930	952530	41.45%	5.402%
6	10.732	1292	1301	1308	rBV	213242	376051	16.36%	2.133%
7	13.188	1711	1719	1726	rBV	1287117	1963899	85.46%	11.137%
8	14.562	1944	1953	1959	rBV	318628	490223	21.33%	2.780%
9	14.815	1990	1996	2004	rBV7	14626	25132	1.09%	0.143%
10	15.920	2178	2184	2189	rBV	56865	83045	3.61%	0.471%
11	16.049	2199	2206	2213	rBV	1006199	1496854	65.14%	8.489%
12	17.306	2414	2420	2425	rBV	374268	544029	23.67%	3.085%
13	17.347	2425	2427	2431	rVV	42178	52241	2.27%	0.296%
14	17.394	2431	2435	2439	rVB3	21561	28578	1.24%	0.162%
15	18.076	2548	2551	2557	rBV3	33815	47658	2.07%	0.270%
16	18.152	2559	2564	2567	rVV4	33103	49099	2.14%	0.278%
17	18.199	2567	2572	2581	rBV	333868	474560	20.65%	2.691%
18	18.517	2619	2626	2634	rBV4	92545	158402	6.89%	0.898%
19	19.210	2741	2744	2751	rBV3	42268	76563	3.33%	0.434%
20	19.357	2766	2769	2775	rVB	144928	212638	9.25%	1.206%
21	19.468	2784	2788	2799	rBV2	142708	237579	10.34%	1.347%
22	19.721	2828	2831	2838	rVB	121103	177091	7.71%	1.004%
23	19.921	2860	2865	2874	rVB	1633650	2297979	100.00%	13.032%
24	20.561	2971	2974	2978	rBV3	109529	143825	6.26%	0.816%
25	21.213	3082	3085	3095	rVB3	200094	306372	13.33%	1.737%
26	21.560	3139	3144	3149	rBV2	319280	533804	23.23%	3.027%
27	22.365	3276	3281	3291	rVB3	234157	508782	22.14%	2.885%
28	23.840	3525	3532	3538	rBV	692996	1456730	63.39%	8.261%
29	25.896	3873	3882	3892	rVB	535677	1661018	72.28%	9.420%

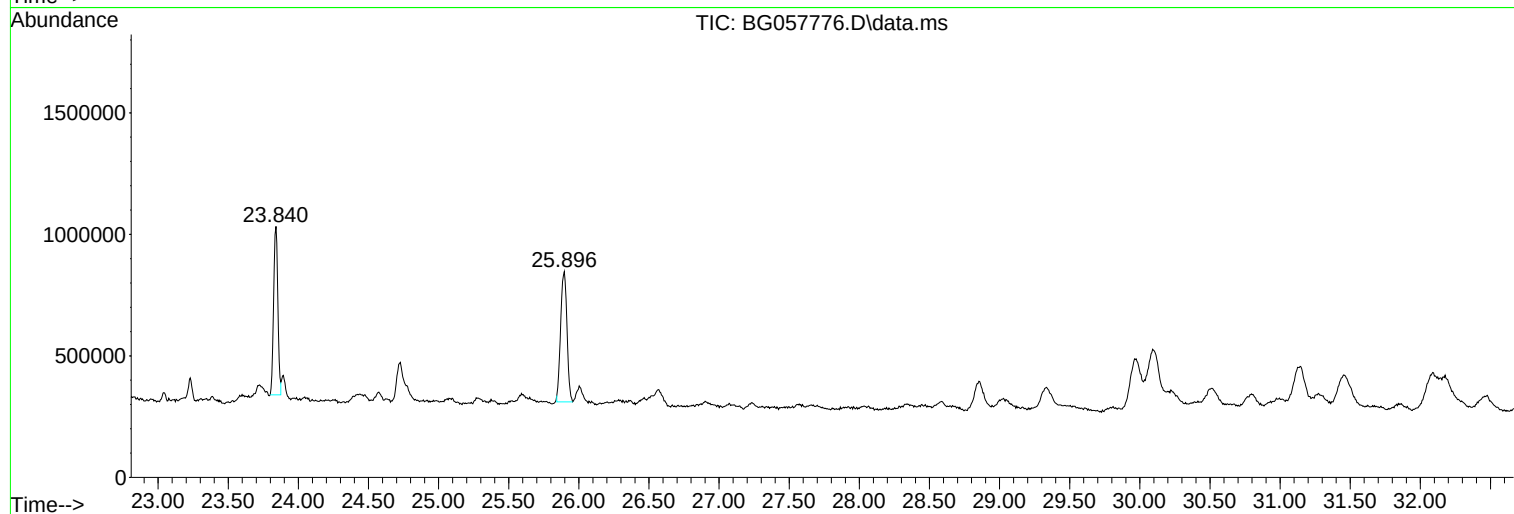
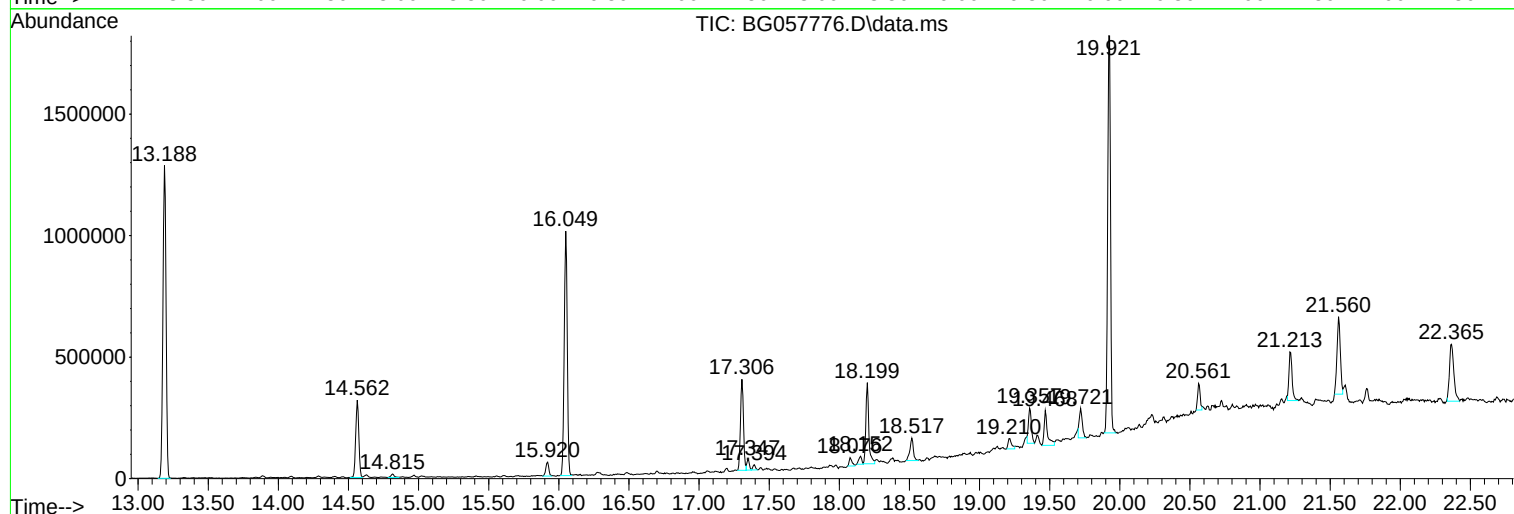
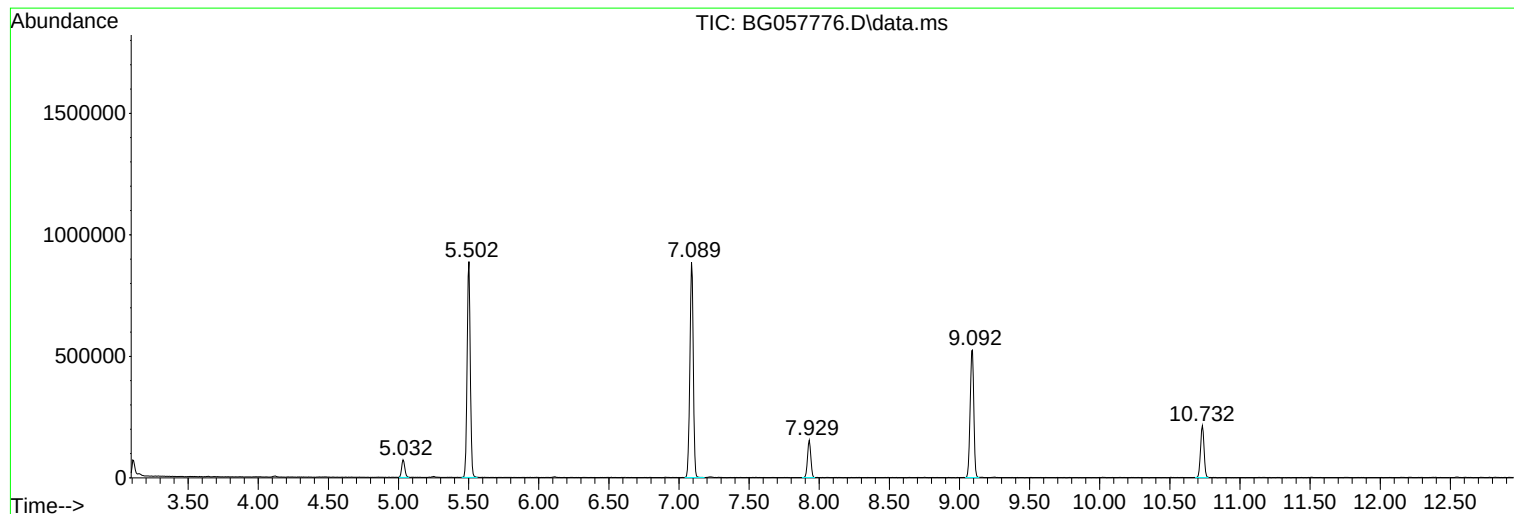
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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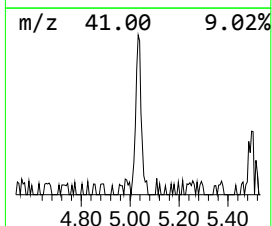
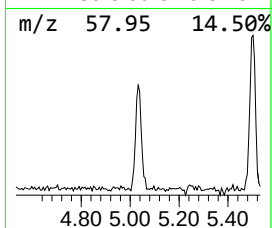
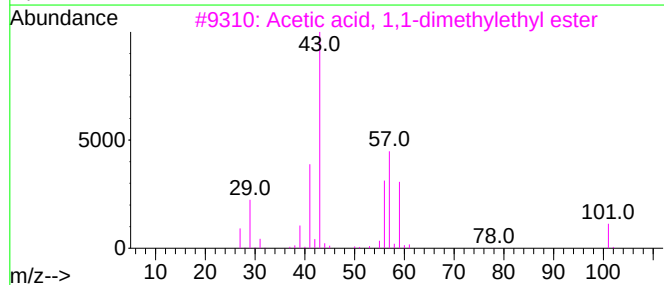
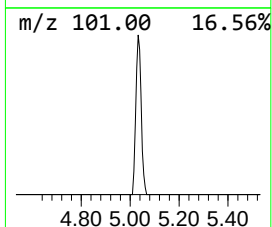
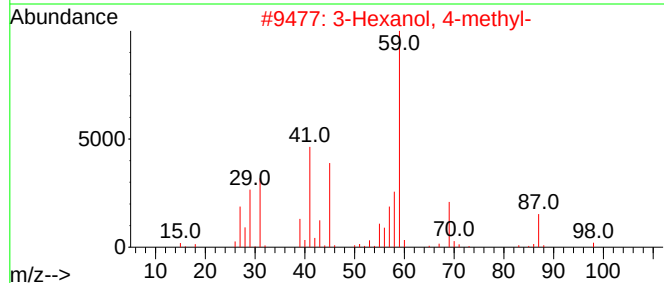
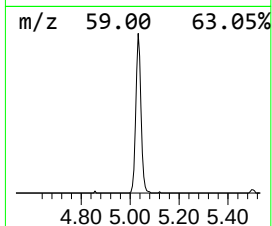
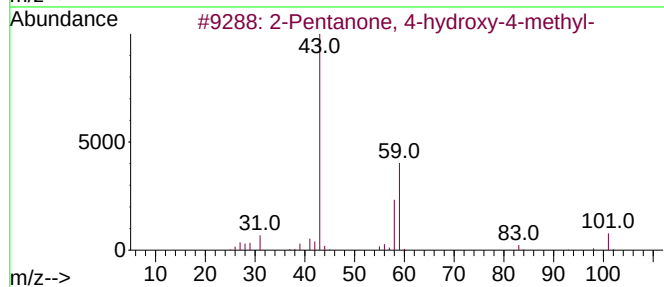
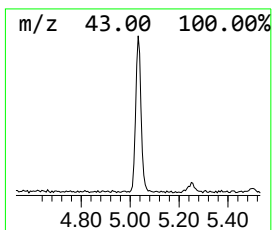
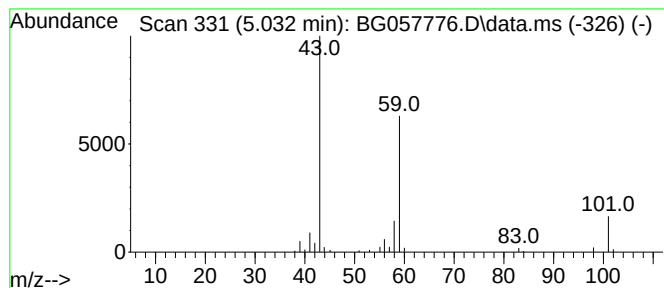
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.032	8.87 ng	112025	1,4-Dichlorobenzene-d4	7.929

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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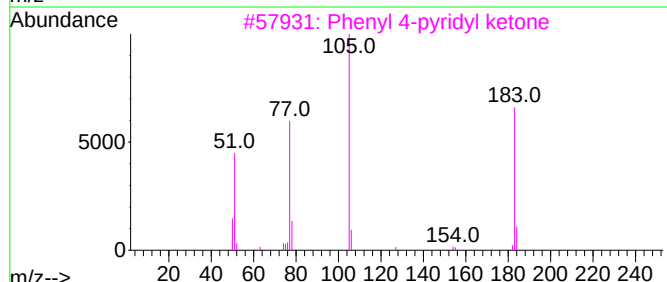
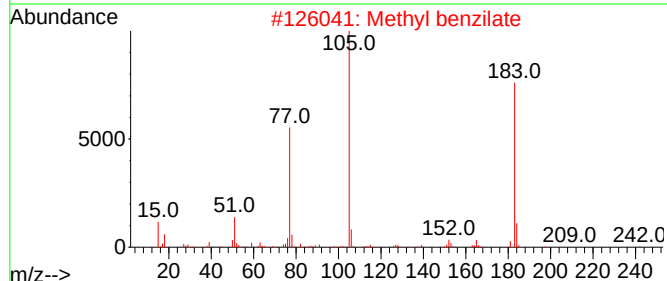
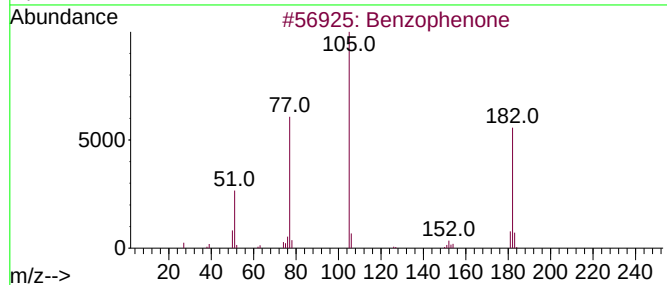
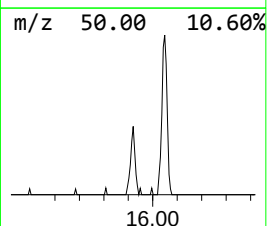
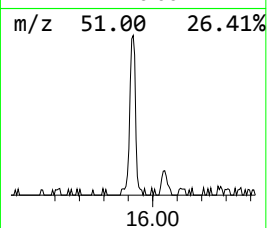
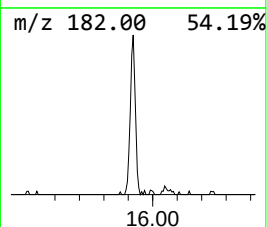
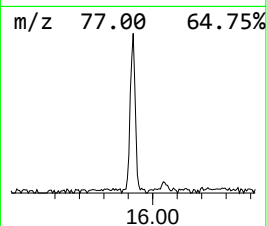
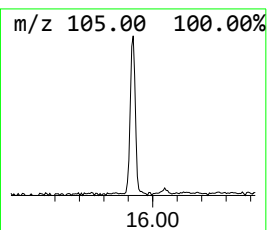
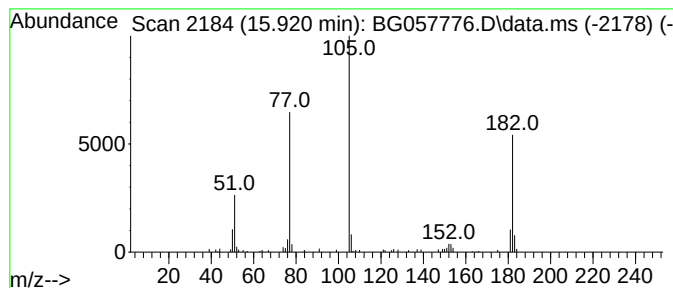
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.920	3.39 ng	83045	Acenaphthene-d10	14.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Methyl benzilate	242	C15H14O3	000076-89-1	47
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
4			Benzilic acid	228	C14H12O3	000076-93-7	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43



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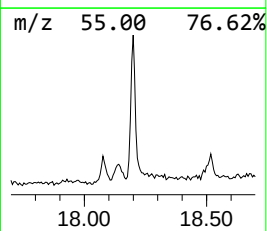
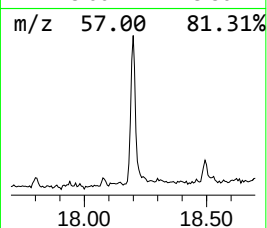
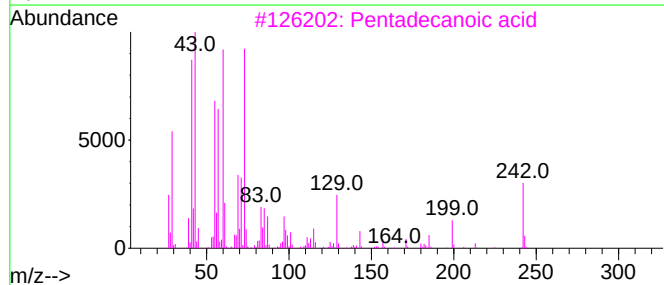
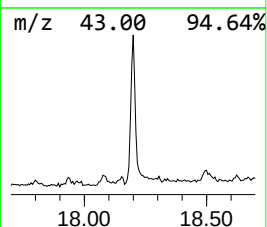
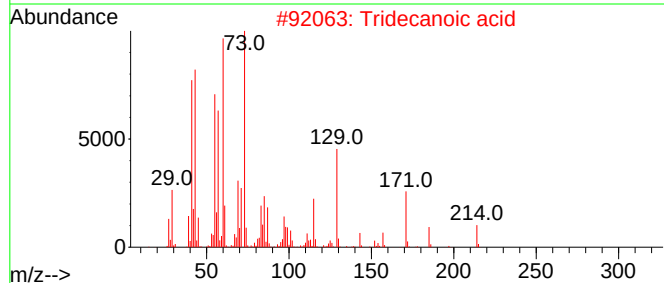
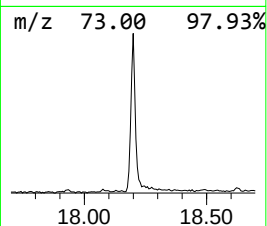
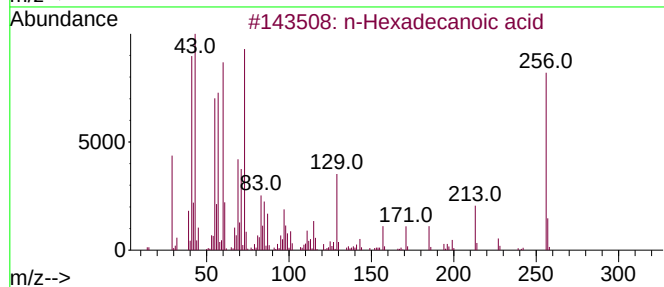
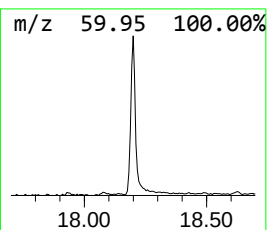
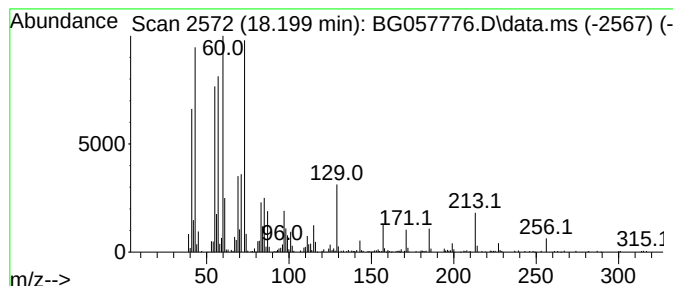
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.199	17.45 ng	474560	Phenanthrene-d10	17.306

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5		Undecanoic acid	186	C11H22O2	000112-37-8	62



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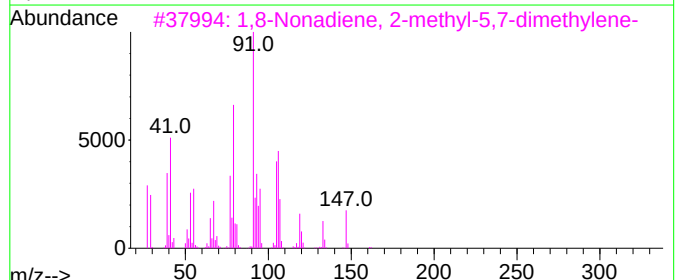
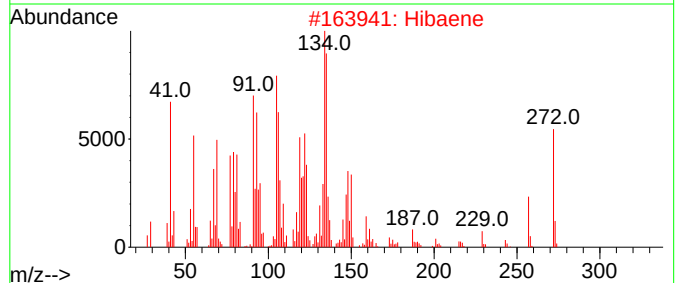
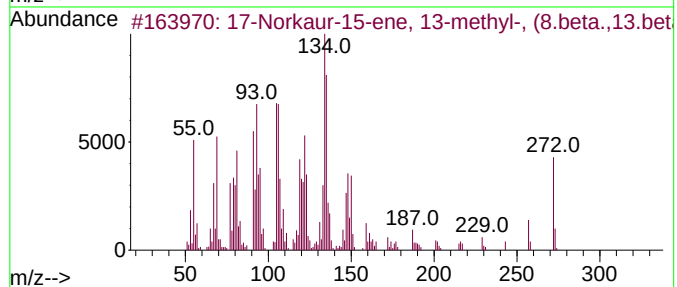
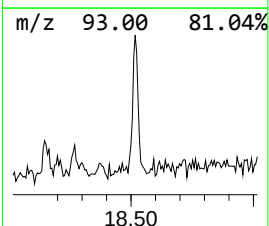
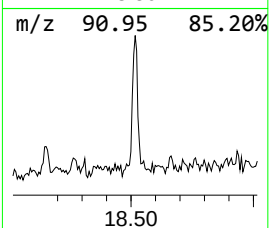
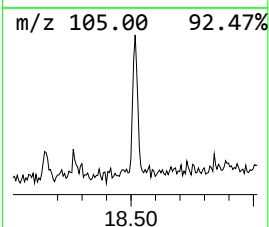
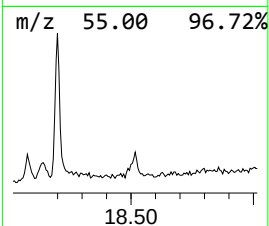
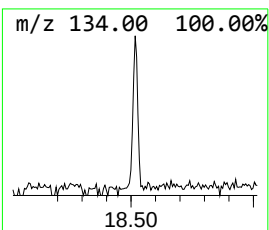
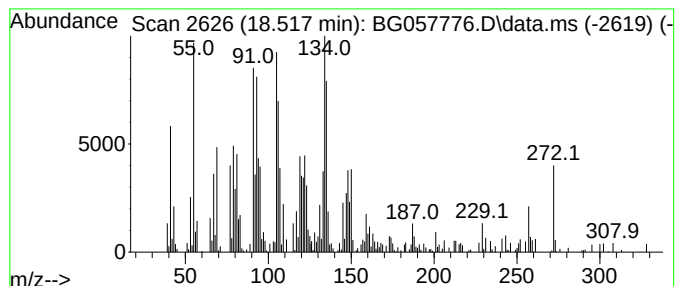
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 17-Norkaur-15-ene, 13-methy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.517	5.82 ng	158402	Phenanthrene-d10	17.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Norkaur-15-ene, 13-methyl-, (...	272	C20H32	003564-54-3	97
2			Hibaene	272	C20H32	002359-73-1	90
3			1,8-Nonadiene, 2-methyl-5,7-dime...	162	C12H18	1000152-68-8	25
4			2-Allylphenol	134	C9H10O	001745-81-9	25
5			Tricyclo[3.3.1.1(3,7)]decane-1-c...	161	C11H15N	023074-42-2	25



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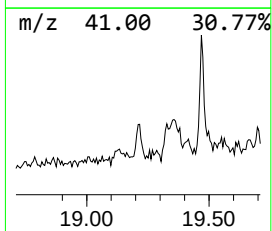
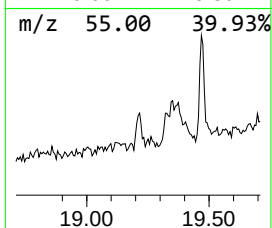
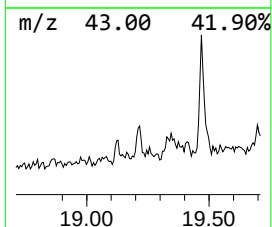
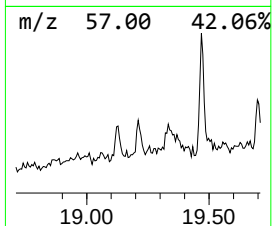
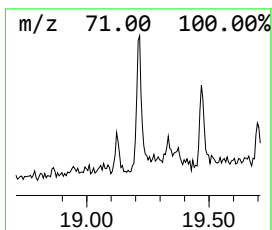
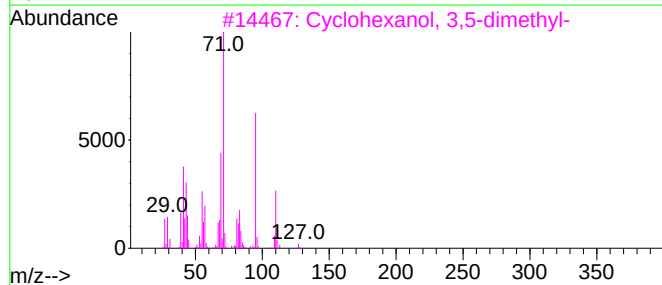
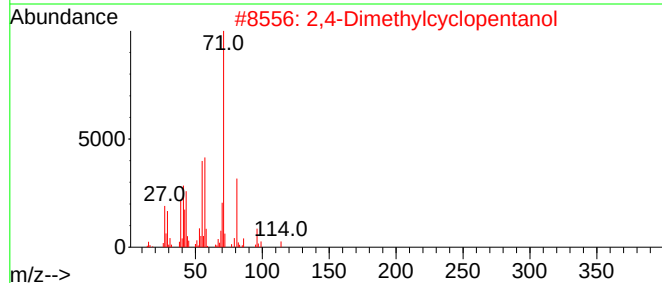
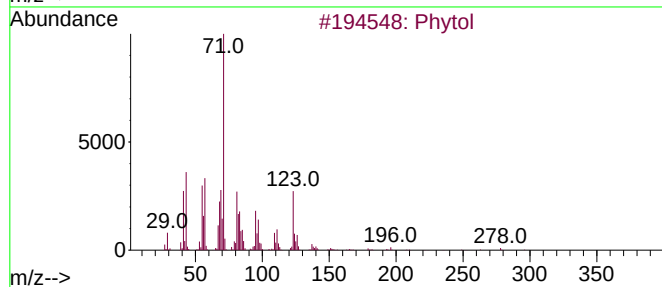
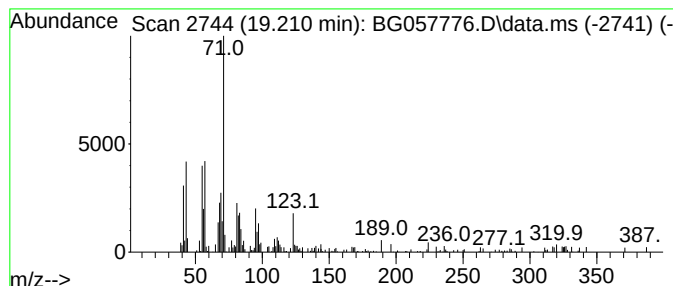
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Phytol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	2.81 ng	76563	Phenanthrene-d10	17.306

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phytol	296	C20H40O	000150-86-7	86
2			2,4-Dimethylcyclopentanol	114	C7H14O	089794-28-5	50
3			Cyclohexanol, 3,5-dimethyl-	128	C8H16O	005441-52-1	47
4			6-Methyl-2-heptanol, 2-methylpro...	200	C12H24O2	1000447-36-7	43
5			Isophytol	296	C20H40O	000505-32-8	43



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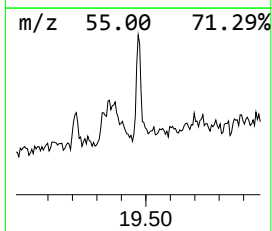
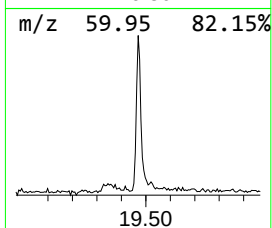
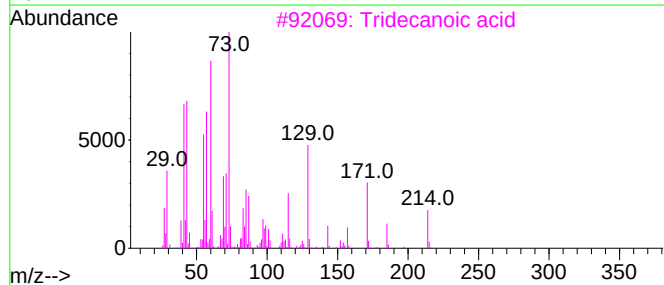
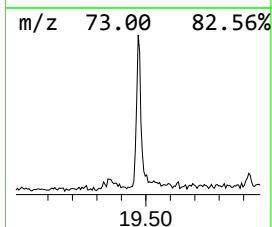
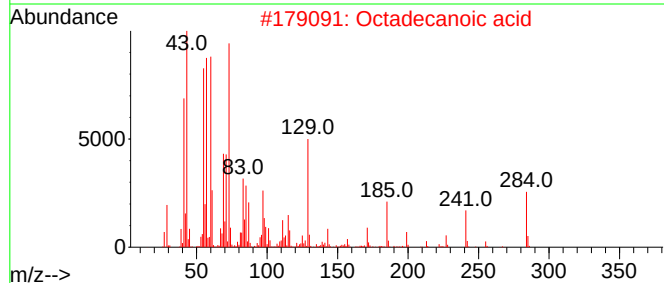
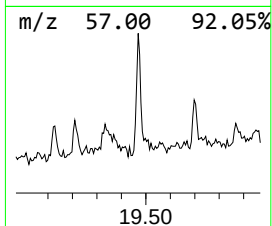
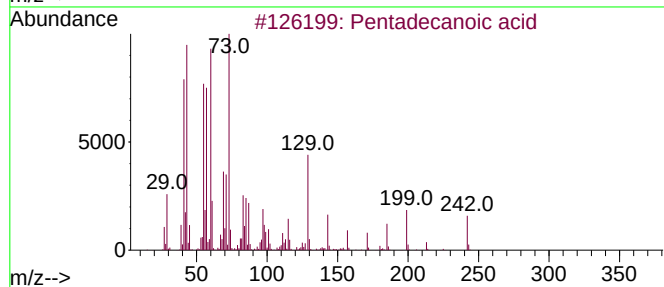
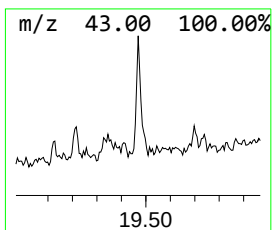
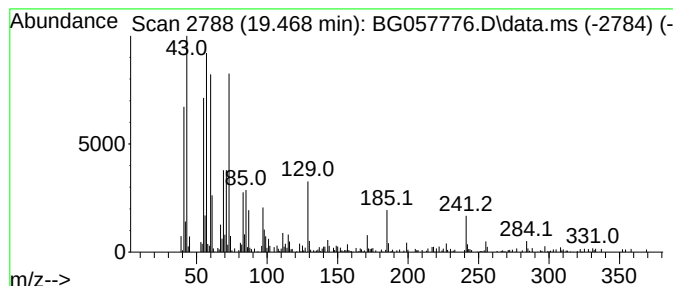
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	8.90 ng	237579	Chrysene-d12	21.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
Operator : CG/JU
Sample : 03287-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OK-1-061523

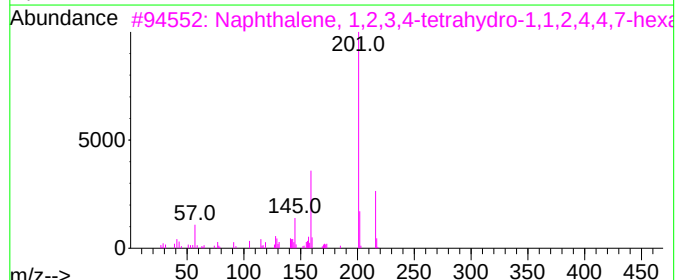
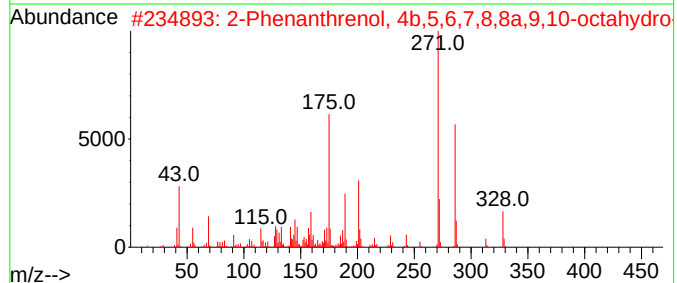
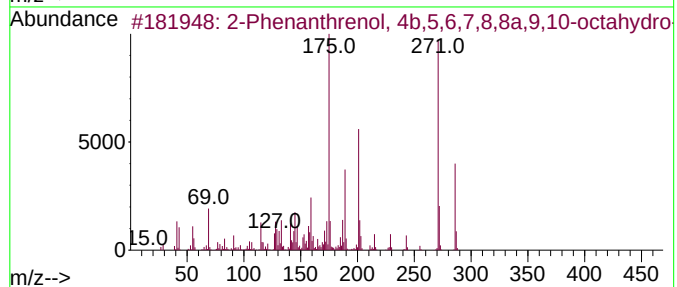
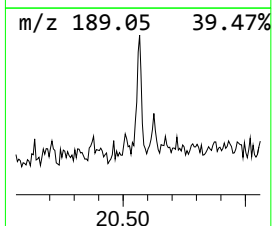
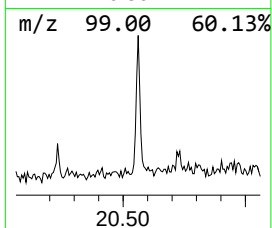
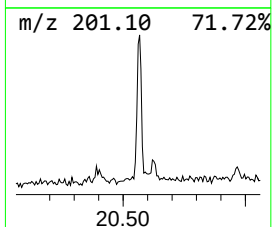
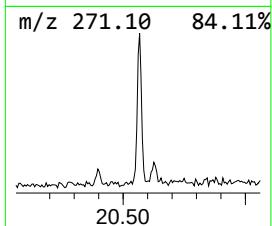
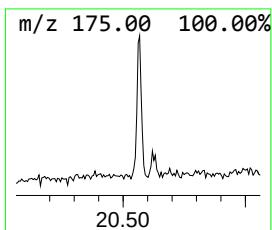
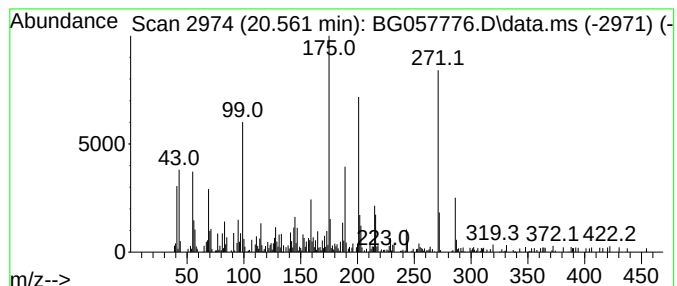
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.561	5.39 ng	143825	Chrysene-d12	21.560

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	80
2		2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	27
3		Naphthalene, 1,2,3,4-tetrahydro...	216	C16H24	002084-69-7	25
4		7-Bromo-[1,2,4]triazolo[1,5-a]py...	284	C9H13BrN4Si	1000507-40-0	22
5		Oxazole, 2-(1-naphthalenyl)-5-ph...	271	C19H13NO	000846-63-9	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
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ClientSampleId :
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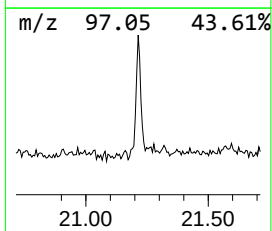
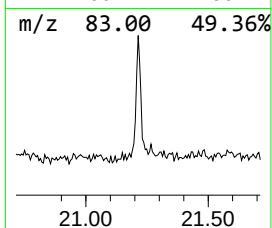
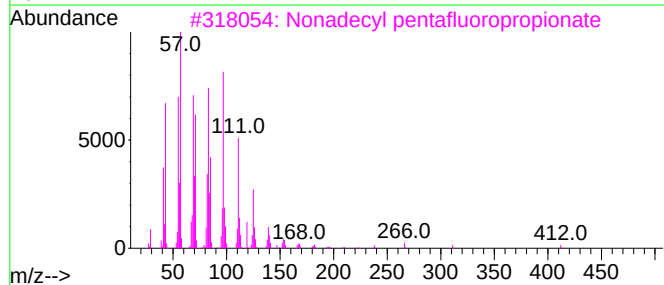
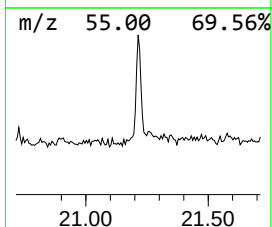
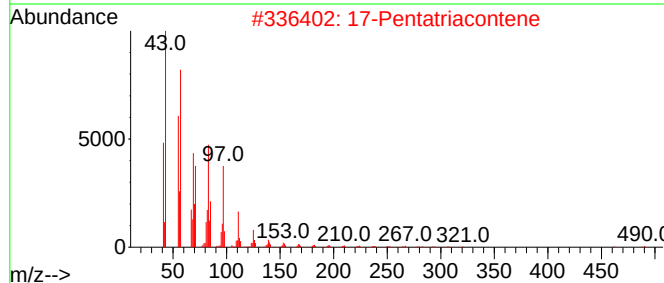
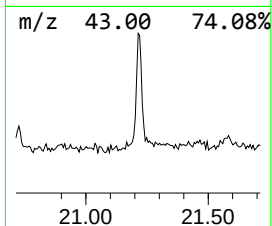
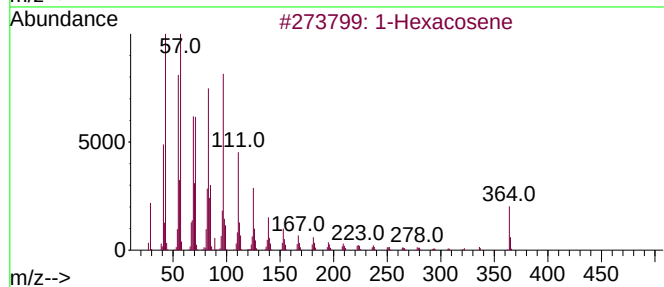
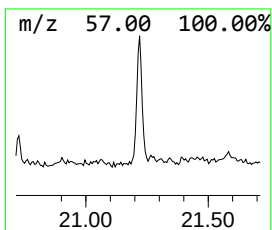
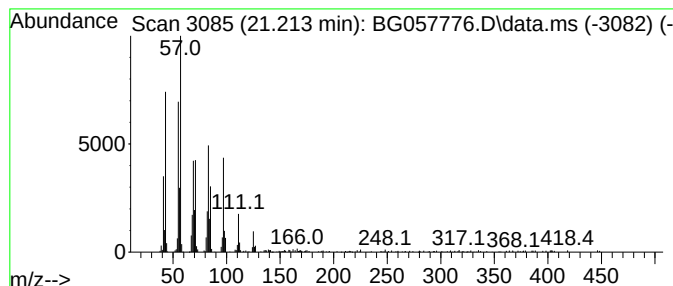
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 1-Hexacosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.214	11.48 ng	306372	Chrysene-d12	21.560

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexacosene	364	C26H52	018835-33-1	93
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	90
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
Operator : CG/JU
Sample : 03287-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
OK-1-061523

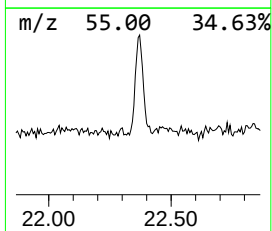
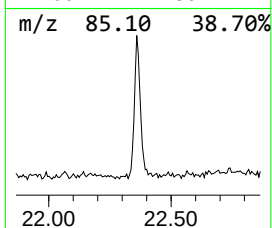
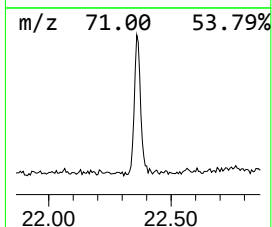
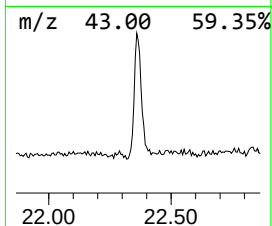
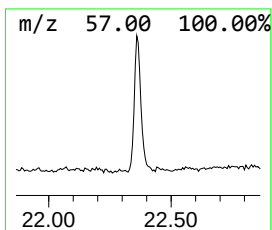
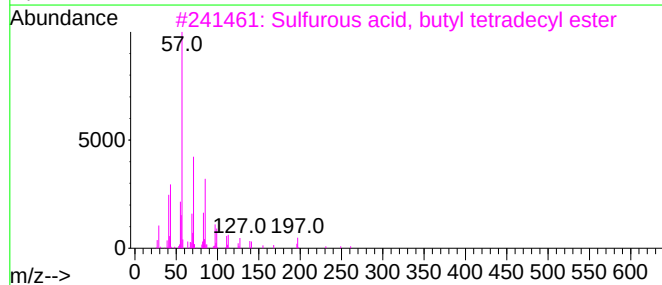
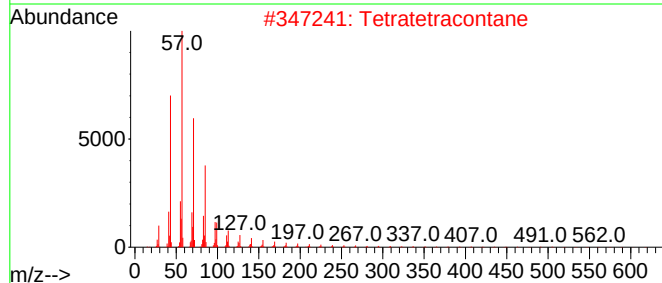
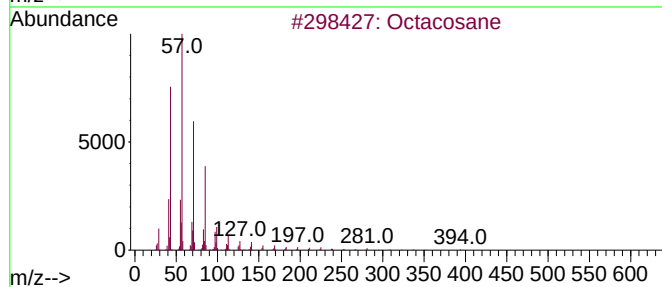
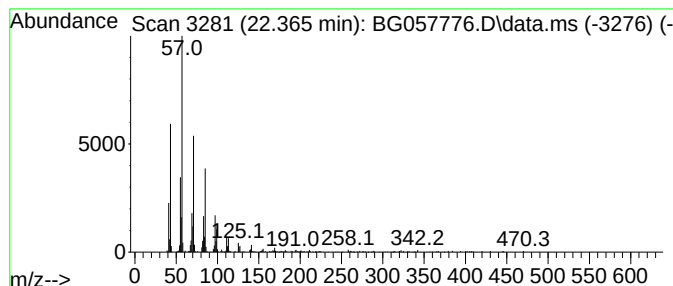
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.365	19.06 ng	508782	Chrysene-d12	21.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	93
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	87
4			Hentriacontane	437	C31H64	000630-04-6	87
5			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
Operator : CG/JU
Sample : 03287-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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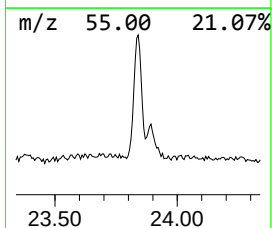
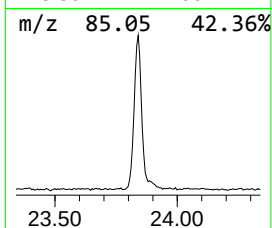
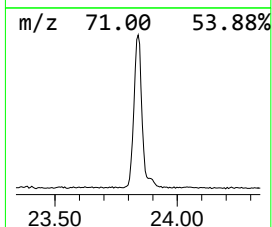
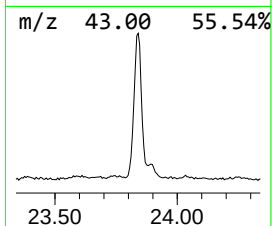
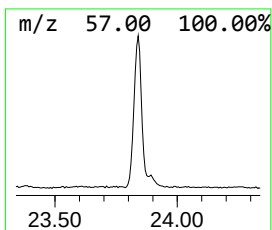
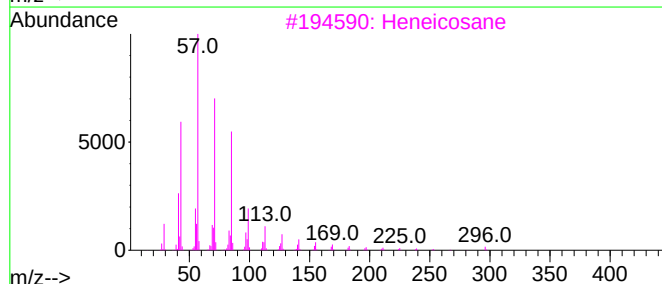
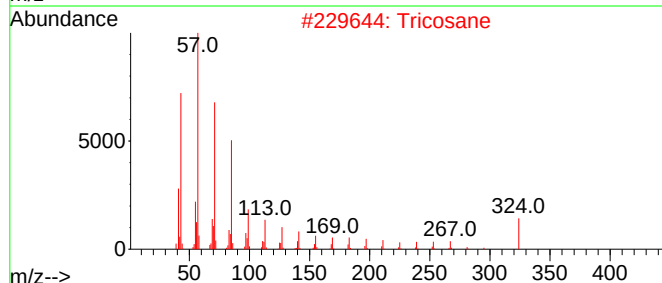
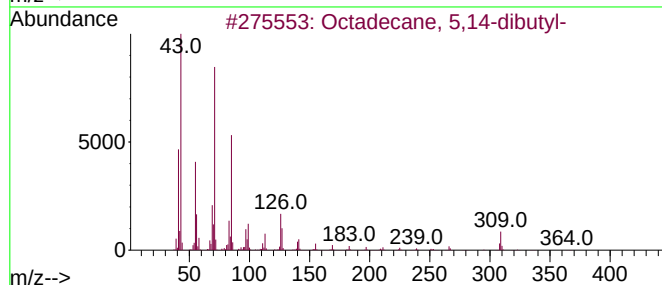
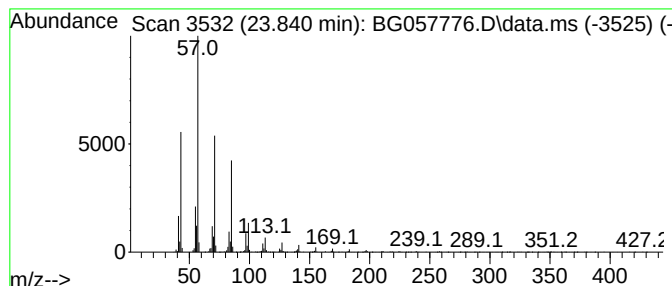
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecane, 5,14-dibutyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.840	20.00 ng	1456730	Perylene-d12	24.721

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	90
2		Tricosane	324	C23H48	000638-67-5	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
Operator : CG/JU
Sample : 03287-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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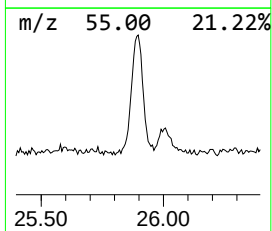
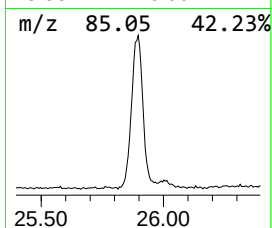
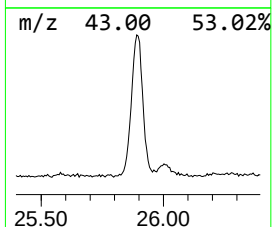
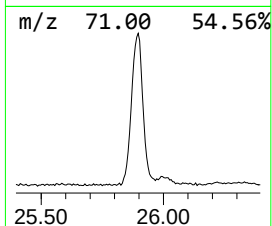
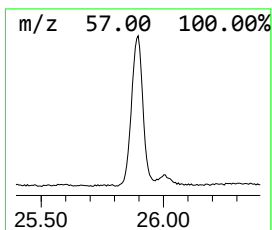
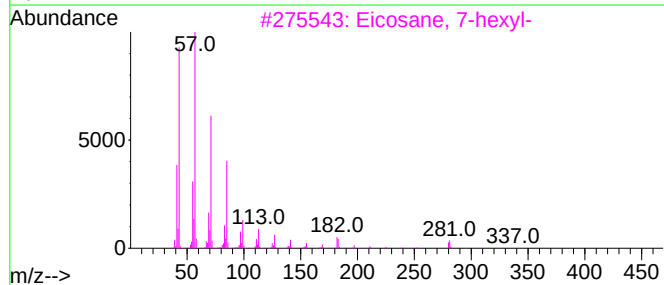
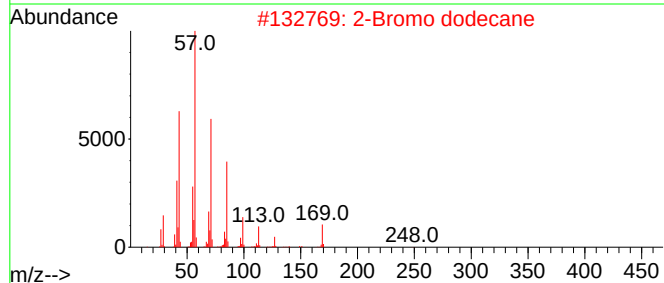
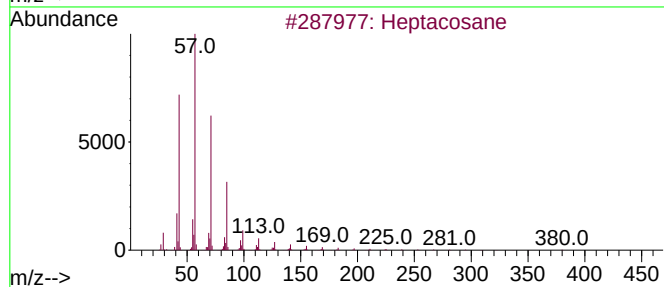
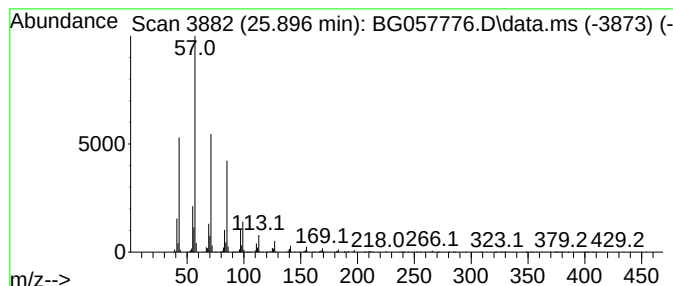
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heptacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.896	22.80 ng	1661020	Perylene-d12	24.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	98
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	91
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4			Pentacosane	352	C25H52	000629-99-2	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062023\
Data File : BG057776.D
Acq On : 20 Jun 2023 14:49
Operator : CG/JU
Sample : 03287-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzophenone	15.920	3.4	ng	83045	3	14.562	490223	20.0
n-Hexadecanoic ...	18.199	17.4	ng	474560	4	17.306	544029	20.0
17-Norkaur-15-e...	18.517	5.8	ng	158402	4	17.306	544029	20.0
Phytol	19.210	2.8	ng	76563	4	17.306	544029	20.0
Pentadecanoic acid	19.468	8.9	ng	237579	5	21.560	533804	20.0
2-Phenanthrenol...	20.561	5.4	ng	143825	5	21.560	533804	20.0
1-Hexacosene	21.214	11.5	ng	306372	5	21.560	533804	20.0
Octacosane	22.365	19.1	ng	508782	5	21.560	533804	20.0
Octadecane, 5,1...	23.840	20.0	ng	1456730	6	24.721	1456730	20.0
Heptacosane	25.896	22.8	ng	1661020	6	24.721	1456730	20.0